Attorney's Docket No.: 14435-004001 / VPI/03-12

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant : Pierce et al.
Serial No. : 10/790,507
Filed : March 1, 2004
Title : TARGET LIGAND GENERATION

Art Unit : 1631
Examiner : Unknown

MAIL STOP AMENDMENT
Commissioner for Patents
P.O. Box 1450
Alexandria, VA 22313-1450

INFORMATION DISCLOSURE STATEMENT

Applicants request consideration of the references listed on the attached PTO-1449 form. Under 37 C.F.R. § 1.98 (a)(2)(ii), only copies of foreign patent documents and/or non-patent literature are enclosed. Copies of any listed U.S. patents or U.S. patent application publications can be provided upon request. A copy of a Search Report dated February 28, 2005, in PCT/US04/06131 is also enclosed.

This statement is being filed before the receipt of a first Office Action on the merits. Please apply any charges or credits to Deposit Account No. 06-1050, referencing attorney docket number 14435-004001.

Respectfully submitted,

Date: 4-29-05

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Substitute Form PTO-1449 (Modified)	U.S. Department of Commerce Patent and Trademark Office	Attorney's Docket No. 14435-004001	Application No. 10/790,507
Information Disclosure Statement by Applicant (Use several sheets if necessary) (37 CFR 1.98(b))		Applicant Pierce et al.	
		Filing Date March 1, 2004	Group Art Unit 1631

U.S. Patent Documents

Examiner Initial	Desig. ID	Document Number	Publication Date	Patentee	Class	Subclass	Filing Date If Appropriate
	AA						

Foreign Patent Documents or Published Foreign Patent Applications

Examiner Initial	Desig. ID	Document Number	Publication Date	Country or Patent Office	Class	Subclass	Translation Yes	Translation No
	AB							

Other Documents (include Author, Title, Date, and Place of Publication)

Examiner Initial	Desig. ID	Document
	AC	Bemis et al. "The Properties of Known Drugs. 1. Molecular Frameworks" *J. Med. Chem.* 39:2887-2893 (1996)
	AD	Böhm et al. "The computer program LUDI: A new method for the de novo design of enzyme inhibitors" *J. Comput.-Aided Mol. Des.* 6:61-78 (1992)
	AE	Brooks et al. "CHARMM: A Program for Macromolecular Energy, Minimization, and Dynamics Calculations" *J. Comput. Chem.* 4:187-217 (1983)
	AF	Charifson et al. "Consensus Scoring: A Method for Obtaining Improved Hit Rates from Docking Databases of Three-Dimensional Structures into Proteins" *J. Med. Chem.* 42:5100-5109 (1999)
	AG	Eldridge et al. "Empirical scoring functions: I. The development of a fast empirical scoring function to estimate the binding affinity of ligands in receptor complexes" *J. Comput.-Aided Mol. Des.* 11:425-445 (1997)
	AH	Ewing et al. "Critical Evaluation of Search Algorithms for Automated Molecular Docking and Database Screening" *J. Comput. Chem.* 18(9):1175-1189 (1997)
	AI	Flower "SERF: A program for accessible surface area calculations" *J. Mol. Graphics Model.* 15:238-244 (1998)
	AJ	Gasteiger et al. "Automatic Generation of 3D-Atomic Coordinates for Organic Molecules" *Tetrahed Comp. Meth.* 3:537-547 (1990)
	AK	Gasteiger et al. "Chemical Information in 3D Space" *J. Chem. Inf. Comput. Sci.* 36:1030-1037 (1996)
	AL	Gehlhaar et al. "Molecular recognition of the inhibitor AG-1343 by HIV-1 protease: conformationally flexible docking by evolutionary programming" *Chem. Bio.* 2:317-324 (1995)
	AM	Guex et al. "SWISS-MODEL and the Swiss-PdbViewer: An environment for comparative protein modeling" *Electrophoresis* 18:2714-2723 (1997)
	AN	Halgren "Merck Molecular Force Field. I. Basis, Form, Scope, Parameterization, and Performance of MMFF94" *J. Comput. Chem.* 17:490-519 (1996)
	AO	Halgren "Merck Molecular Force Field. III. Molecular Geometries and Vibrational Frequencies for MMFF94" *J. Comput. Chem.* 17:553-586 (1996)
	AP	Halgren "Merck Molecular Force Filed. II. MMFF94 van der Waals and Electrostatic Parameters for Intermolecular Interactions" *J. Comput. Chem.* 17:520-552 (1996)
	AQ	Ho et al. "SPLICE: A program to assemble partial query solutions from three-dimensional database searches into novel ligands" *J. of Computer-Aided Mol. Desig.* 7:623-647 (1993)

Examiner Signature	Date Considered

EXAMINER: Initials citation considered. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.

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Other Documents (include Author, Title, Date, and Place of Publication)		
Examiner Initial	Desig. ID	Document
	AR	Holm et al. "Protein Structure Comparison by Alignment of Distance Matrices" *Mol. Biol.* 233:123-138 (1993)
	AS	Honig et al. "Classical Electrostatics in Biology and Chemistry" *Science* 268:1144-1149 (1995)
	AT	Jones et al. "Development and Validation of a Genetic Algorithm for Flexible Docking" *J. Mol. Biol.* 267(3):727-748 (1997)
	AU	Jorgensen et al. "Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids" *J. Am. Chem. Soc.* 118:11225 (1996)
	AV	Klabunde et al. "Drug Design Strategies for Targeting G-Protein-Coupled Receptors" *Chem. Bio. Chem.* 3:928-944 (2002)
	AW	Kleywegt et al. "Detecting Folding Motifs and Similarities in Protein Structures" *Meth. Enzymol.* 277:525-545 (1997)
	AX	Kollman "Free Energy Calculations: Applications to Chemical and Biochemical Phenomena" *Chem. Rev.* 93:2395-2417 (1993)
	AY	Lehtonen et al. "Finding Local Structural Similarities Among Families of Unrelated Protein Structures: A Generic Non-Linear Alignment Algorithm" *Proteins* 34:341-355 (1999)
	AZ	Lemmen et al. "Computational methods for the structural alignment of molecules" *J. Comp-Aided Molec. Des.* 14:215-232 (2000)
	AAA	Lybrand "Ligand-protein docking and rational drug design" *Current Opin. in Structural Biol.* 5:224-228 (1995)
	ABB	Madej et al. "Threading a Database of Protein Cores" *Proteins* 23:356-369 (1995)
	ACC	Meng et al. "Automated Docking with Grid-Based Energy Evaluation" *J. Comp. Chem.* 13:505-524 (1992)
	ADD	Miller et al. "FLOG: A system to select 'quasi-flexible' ligands complementary to a receptor of known three dimensional structure" *J. Comput-Aided Mol. Des.* 8:153-174 (1994)
	AEE	Murray et al. "Empirical scoring functions. II. The testing of an empirical scoring function for the prediction of ligand-receptor binding affinities and the use of Bayesian regression to improve the quality of the model" *J. Comput-Aided Mol. Design* 12:503-519 (1998)
	AFF	Pierce et al. "Kinase Inhibitors and the Case for CH···O Hydrogen Bonds in Protein-Ligand Binding" *Proteins* 49:567-576 (2002)
	AGG	Russell "Detection of Protein Three-dimensional Side-chain Patterns: New Examples of Convergent Evolution" *J. Mol. Biol.* 279:1211-1227 (1998)
	AHH	Schmitt et al. "A New Method to Detect Related Function Among Proteins Independent of Sequence and Fold Homology" *J. Mol. Biol.* 323:387-406 (2002)
	AII	Shindyalov et al. "Protein structure alignment by incremental combinatorial extension (CE) of the optimal path" *Protein Engin.* 11(9):739-747 (1998)
	AJJ	Shoichet et al. "Molecular Docking Using Shape Descriptors" *J. Comput. Chem.* 13:380-397 (1992)
	AKK	Stouch et al. "A Simple Method for the Representation, Quantification, and Comparison of the Volumes and Shapes of Chemical Compounds" *J. Chem. Inf. Comput. Sci.* 26:4-12 (1986)
	ALL	Walters et al. "Prediction of 'drug-likeness'" *Adv. Drug Deliv. Rev.* 54(3):255-271 (2002)
	AMM	Walters et al. "Recognizing molecules with drug-like properties" *Curr. Opin. Chem. Biol.* 3(4):384-387 (1999)

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	ANN	Walters et al. "Virtual screening – an overview" *Drug. Disc. Today* 3:160-178 (1998)
	AOO	Weininger et al. "SMILES. 2. Algorithm for Generation of Unique SMILES Notation" *J. Chem. Inf. Comput. Sci.* 29:97-101 (1989)
	APP	Yamada et al. "Structure-Function Analysis of Vitamin D and VDR Model" *Curr. Pharm. Des.* 6:733-748 (2000)

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